

Parallel Thinking

CSCI 4239/5239

Advanced Computer Graphics

Spring 2024

Objective

- To provide you with a framework based on the techniques and best practices used by experienced parallel programmers for
 - Thinking about the problem of parallel programming
 - Discussing your work with others
 - Addressing performance and functionality issues in your parallel program
 - Using or building useful tools and environments
 - understanding case studies and projects

The Goal

- Speedup $S = T_1 / T_n \sim n$
- Efficiency $E = T_1 / nT_n \sim 1$
- Very hard to achieve
 - Instead of solving the problem in $1/n$ 'th the time, solve a problem n times larger in the same amount of time

Fundamentals of Parallel Computing

- Parallel computing requires that
 - The problem can be decomposed into sub-problems that can be safely solved at the same time
 - The programmer structures the code and data to solve these sub-problems concurrently
- The goals of parallel computing are
 - To solve problems in less time, and/or
 - To solve bigger problems, and/or
 - To achieve better solutions

The problems must be large enough to justify parallel computing and to exhibit exploitable concurrency.

A Recommended Reading

Mattson, Sanders, Massingill, *Patterns for Parallel Programming*, Addison Wesley, 2005, ISBN 0-321-22811-1.

- We draw quite a bit from the book
- A good overview of challenges, best practices, and common techniques in all aspects of parallel programming

Key Parallel Programming Steps

- **To find the concurrency in the problem**
- To structure the algorithm so that concurrency can be exploited
- To implement the algorithm in a suitable programming environment
- To execute and tune the performance of the code on a parallel system

Unfortunately, these have not been separated into levels of abstractions that can be dealt with independently.

Challenges of Parallel Programming

- Finding and exploiting concurrency often requires looking at the problem from a non-obvious angle
 - Computational thinking (J. Wing)
- Dependences need to be identified and managed
 - The order of task execution may change the answers
 - Obvious: One step feeds result to the next steps
 - Subtle: numeric accuracy may be affected by ordering steps that are logically parallel with each other
- Performance can be drastically reduced by many factors
 - Overhead of parallel processing
 - Load imbalance among processor elements
 - Inefficient data sharing patterns
 - Saturation of critical resources such as memory bandwidth

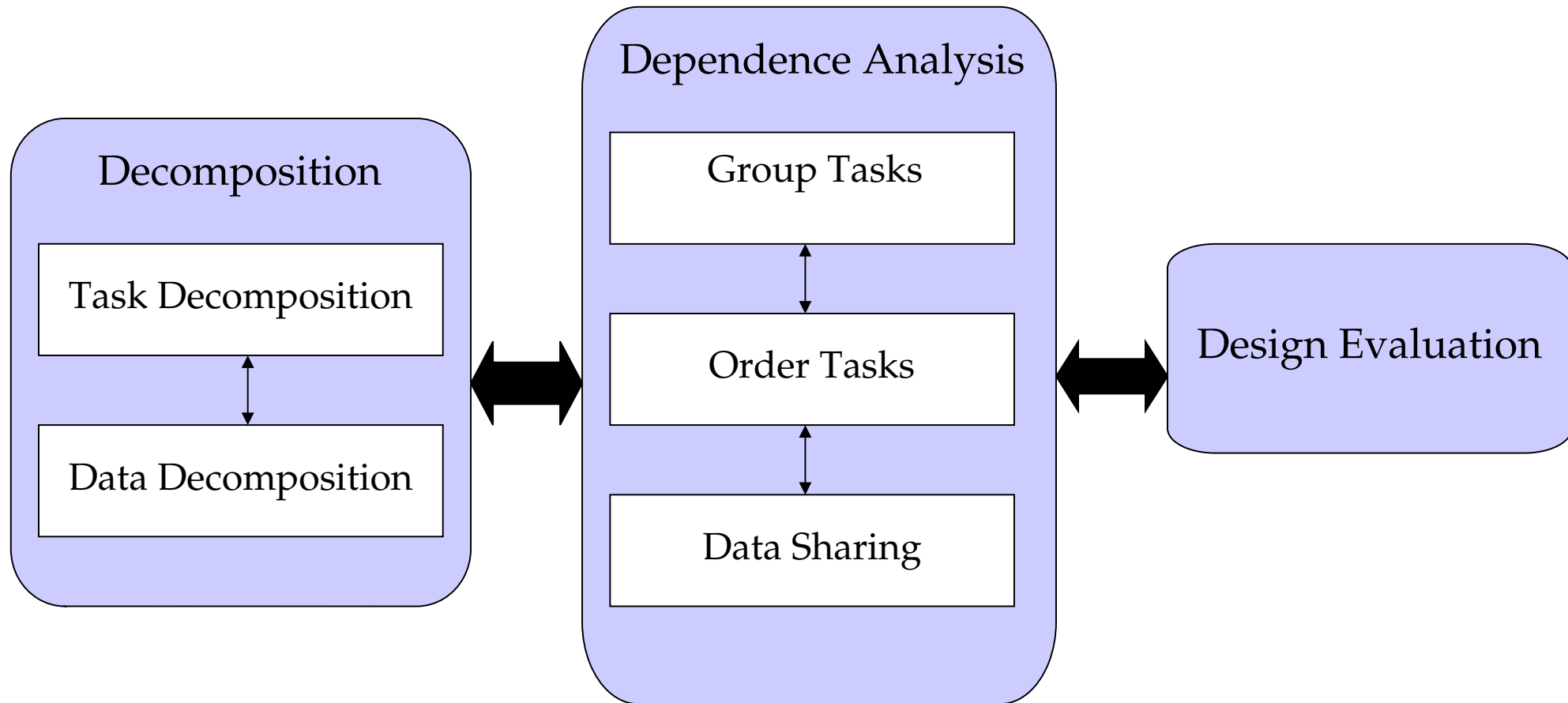
Shared Memory vs. Message Passing

- We will focus on shared memory parallel programming
 - This is what CUDA is based on
 - Future massively parallel microprocessors are expected to support shared memory at the chip level
- The programming considerations of message passing model is quite different!
 - Look at MPI (Message Passing Interface) and its relatives such as Charm++

Finding Concurrency in Problems

- Identify a decomposition of the problem into sub-problems that can be solved simultaneously
 - A **task decomposition** that identifies tasks for potential concurrent execution
 - A **data decomposition** that identifies data local to each task
 - A way of **grouping** tasks and **ordering** the groups to satisfy temporal constraints
 - An analysis on the data **sharing patterns** among the concurrent tasks
 - A **design evaluation** that assesses of the quality the choices made in all the steps

Finding Concurrency - The Process



This is typically an iterative process. Opportunities exist for dependence analysis to play an earlier role in decomposition.

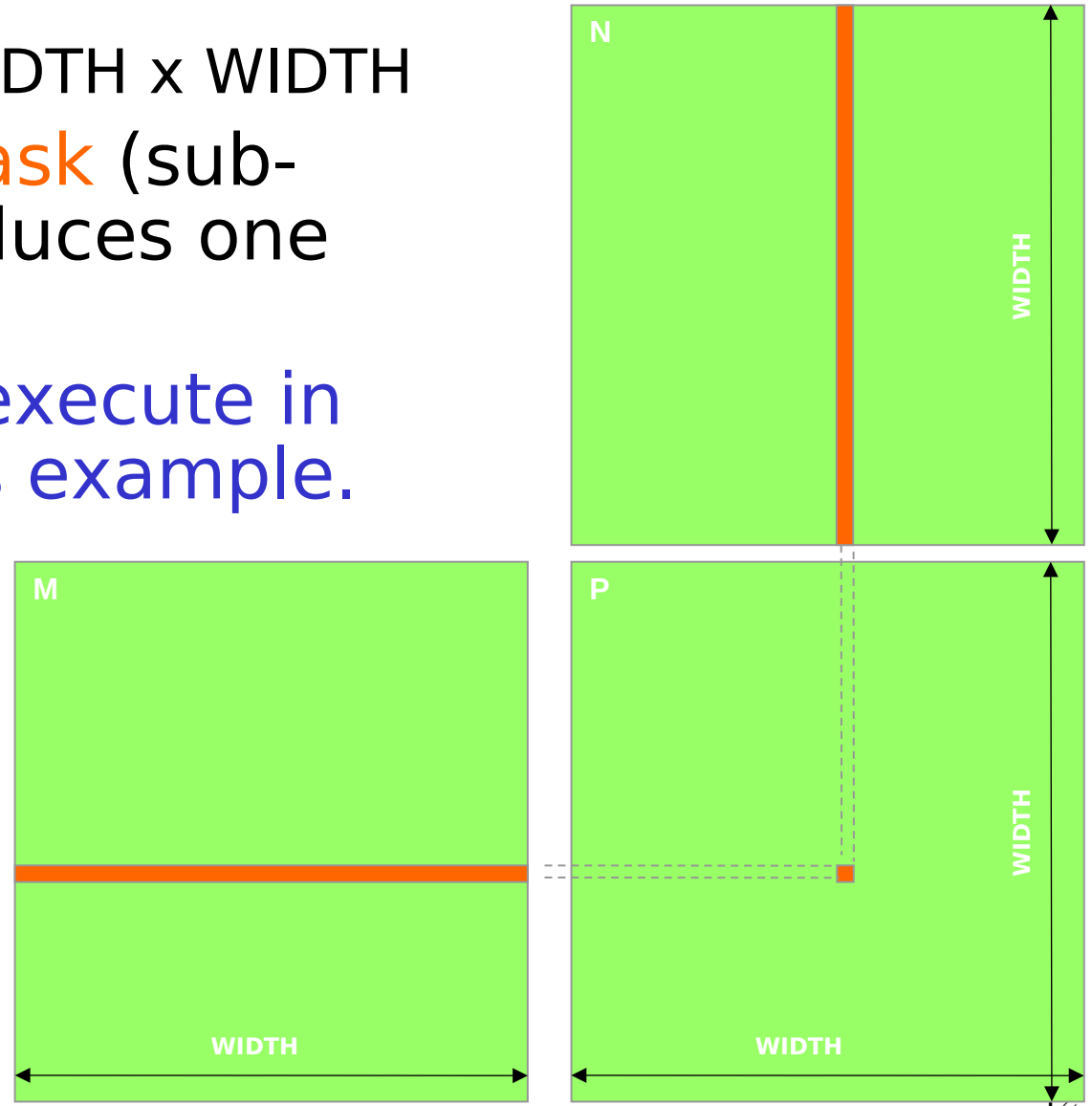
Task Decomposition

- Many large problems can be naturally decomposed into tasks - CUDA kernels are largely tasks
 - The number of tasks used should be adjustable to the execution resources available.
 - Each task must include sufficient work in order to compensate for the overhead of managing their parallel execution.
 - Tasks should maximize reuse of sequential program code to minimize effort.

“In an ideal world, the compiler would find tasks for the programmer. Unfortunately, this almost never happens.”
- Mattson, Sanders, Massingill

Task Decomposition Example - Square Matrix Multiplication

- $P = M * N$ of WIDTH x WIDTH
 - One natural **task** (sub-problem) produces one element of P
 - All tasks can execute in parallel in this example.

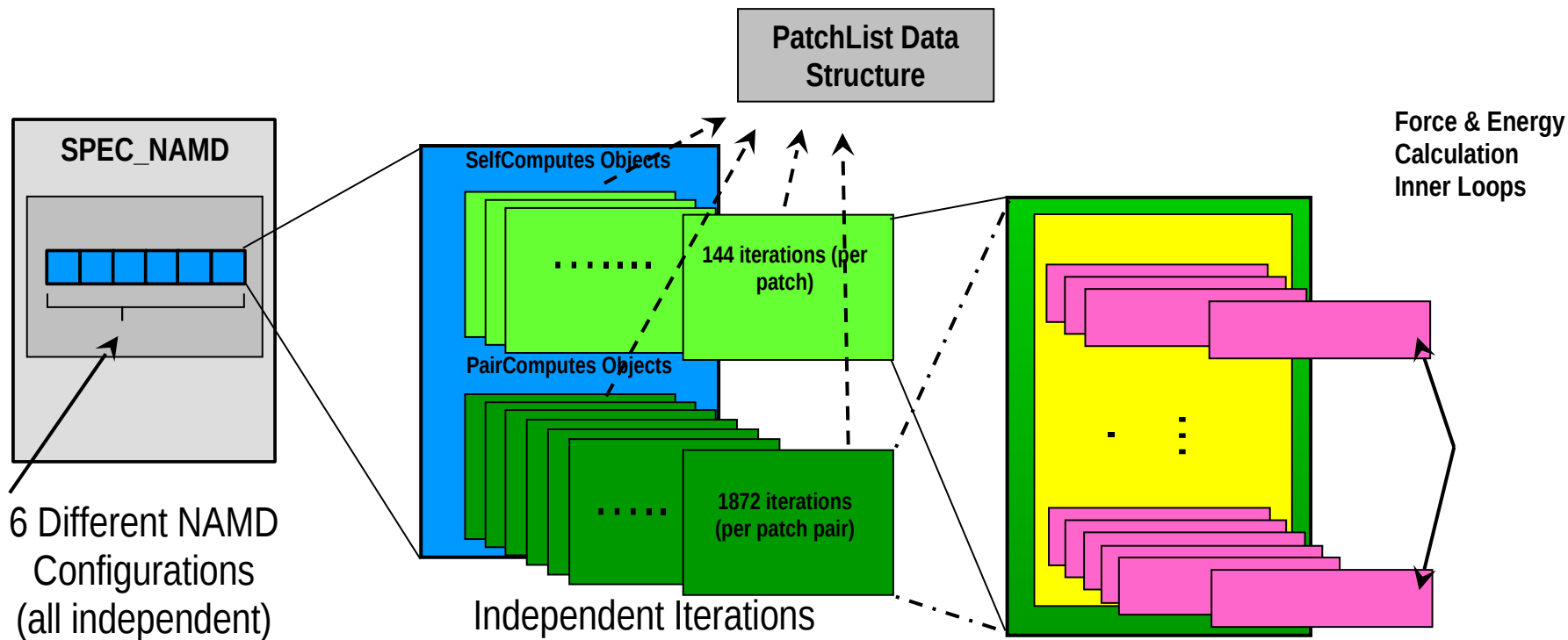


Task Decomposition Example - Molecular Dynamics

- Simulation of motions of a large molecular system
- For each atom, there are natural tasks to calculate
 - Vibrational forces
 - Rotational forces
 - Neighbors that must be considered in non-bonded forces
 - Non-bonded forces
 - Update position and velocity
 - Misc physical properties based on motions
- Some of these can go in parallel for an atom

It is common that there are multiple ways to decompose any given problem.

NAMD

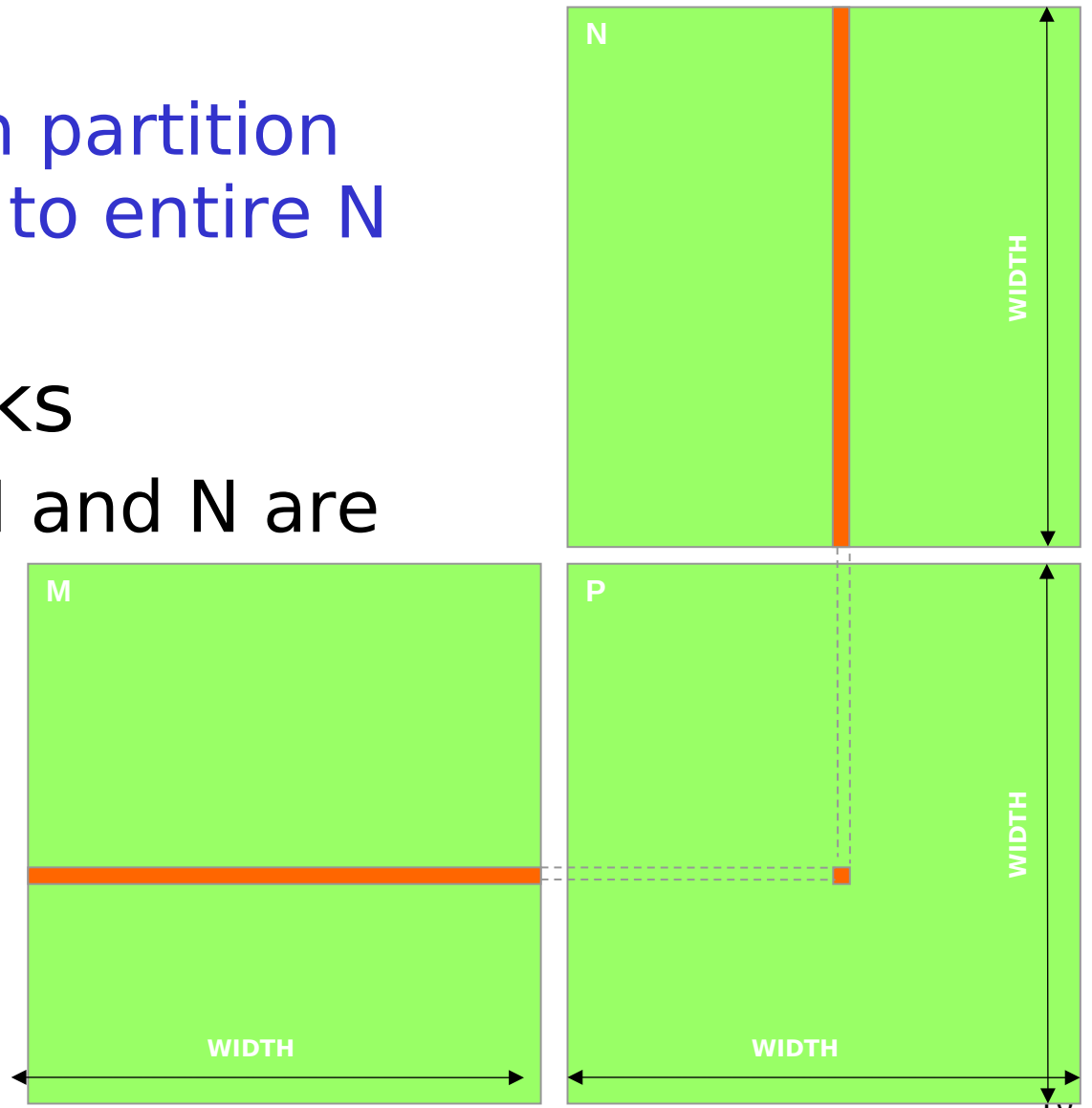


Data Decomposition

- The most compute intensive parts of many large problem manipulate a large data structure
 - Similar operations are being applied to different parts of the data structure, in a mostly independent manner.
 - This is what CUDA is optimized for.
- The data decomposition should lead to
 - Efficient **data usage** by tasks within the partition
 - Few dependencies across the tasks that work on different partitions
 - Adjustable partitions that can be varied according to the hardware characteristics

Data Decomposition Example - Square Matrix Multiplication

- Row blocks
 - Computing each partition requires access to entire N array
- Square sub-blocks
 - Only bands of M and N are needed

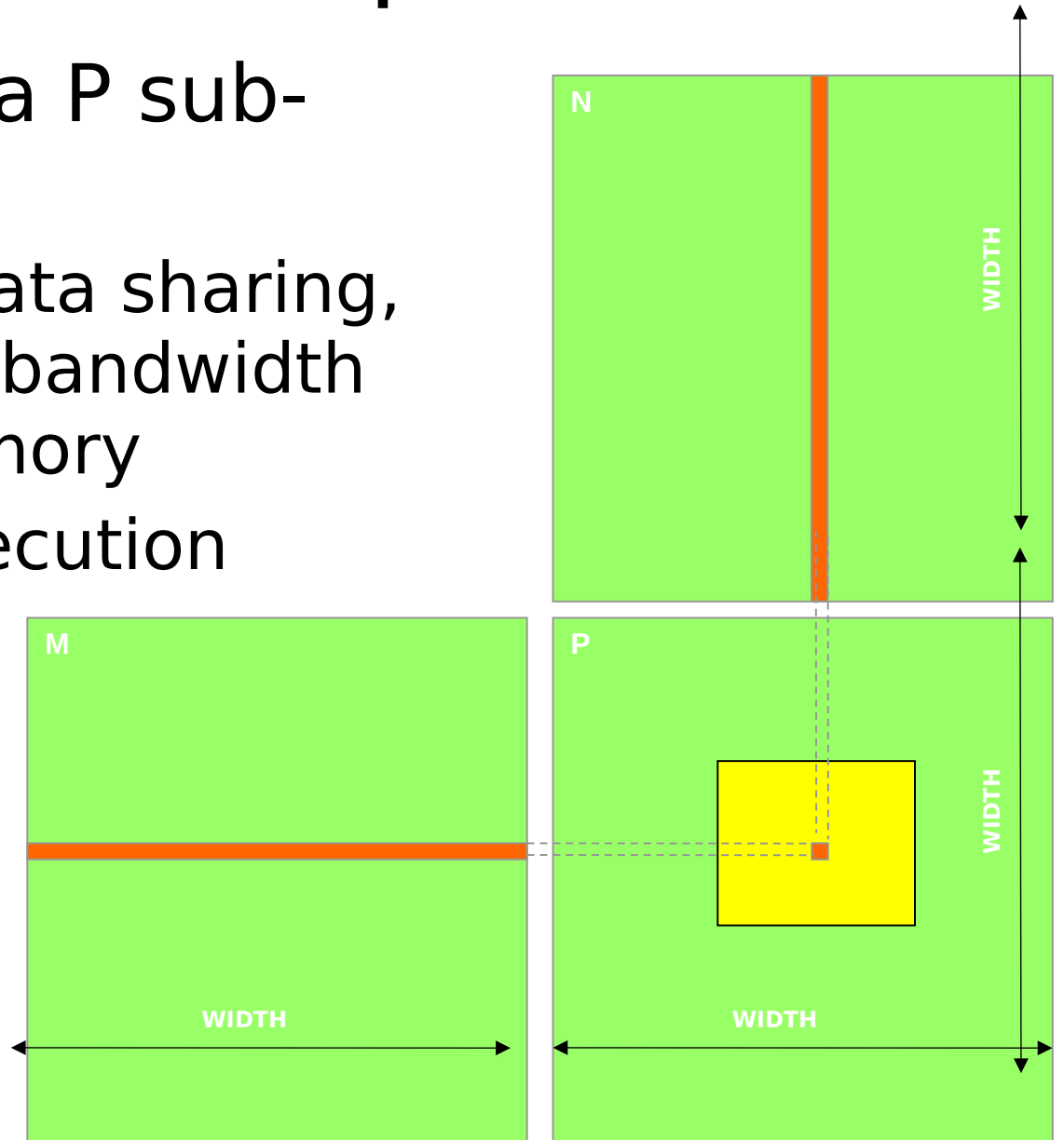


Tasks Grouping

- Sometimes natural tasks of a problem can be grouped together to improve efficiency
 - Reduced synchronization overhead – all tasks in the group can use a barrier to wait for a common dependence
 - All tasks in the group efficiently share data loaded into a common on-chip, shared storage (Shard Memory)
 - Grouping and merging dependent tasks into one task reduces need for synchronization
 - CUDA thread blocks are task grouping examples.

Task Grouping Example - Square Matrix Multiplication

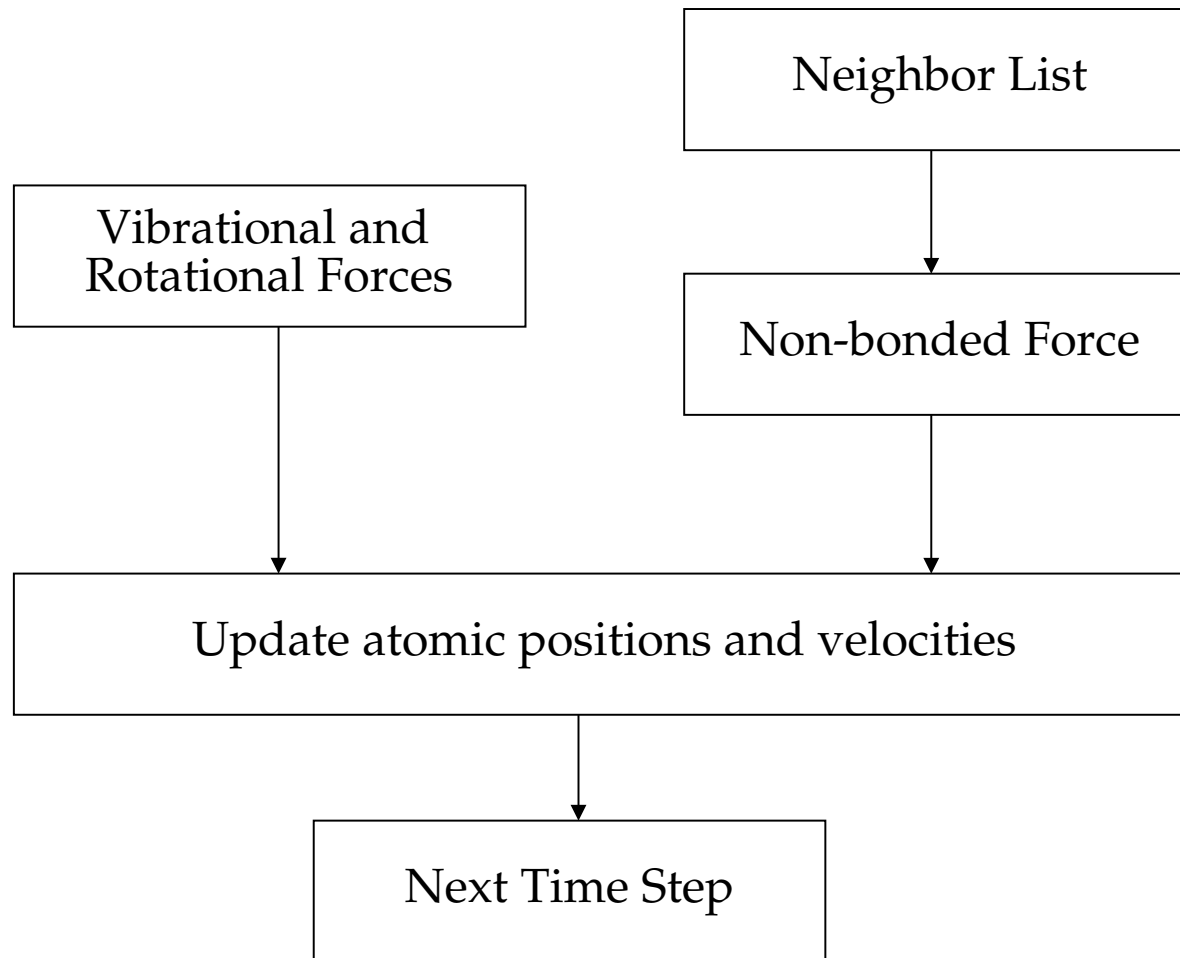
- Tasks calculating a P sub-block
 - Extensive input data sharing, reduced memory bandwidth using Shared Memory
 - All synched in execution



Task Ordering

- Identify the data and resource required by a group of tasks before they can execute them
 - Find the task group that creates it
 - Determine a temporal order that satisfy all data constraints

Task Ordering Example: Molecular Dynamics



Data Sharing

- Data sharing can be a double-edged sword
 - Excessive data sharing can drastically reduce advantage of parallel execution
 - Localized sharing can improve memory bandwidth efficiency
- Efficient memory bandwidth usage can be achieved by synchronizing the execution of task groups and coordinating their usage of memory data
 - Efficient use of on-chip, shared storage
- Read-only sharing can usually be done at much higher efficiency than read-write sharing, which often requires synchronization

Data Sharing Example - Matrix Multiplication

- Each task group will finish usage of each sub-block of N and M before moving on
 - N and M sub-blocks loaded into Shared Memory for use by all threads of a P sub-block
 - Amount of on-chip Shared Memory strictly limits the number of threads working on a P sub-block
- Read-only shared data can be more efficiently accessed as Constant or Texture data

Data Sharing Example - Molecular Dynamics

- The atomic coordinates
 - Read-only access by the neighbor list, bonded force, and non-bonded force task groups
 - Read-write access for the position update task group
- The force array
 - Read-only access by position update group
 - Accumulate access by bonded and non-bonded task groups
- The neighbor list
 - Read-only access by non-bonded force task groups
 - Generated by the neighbor list task group

Key Parallel Programming Steps

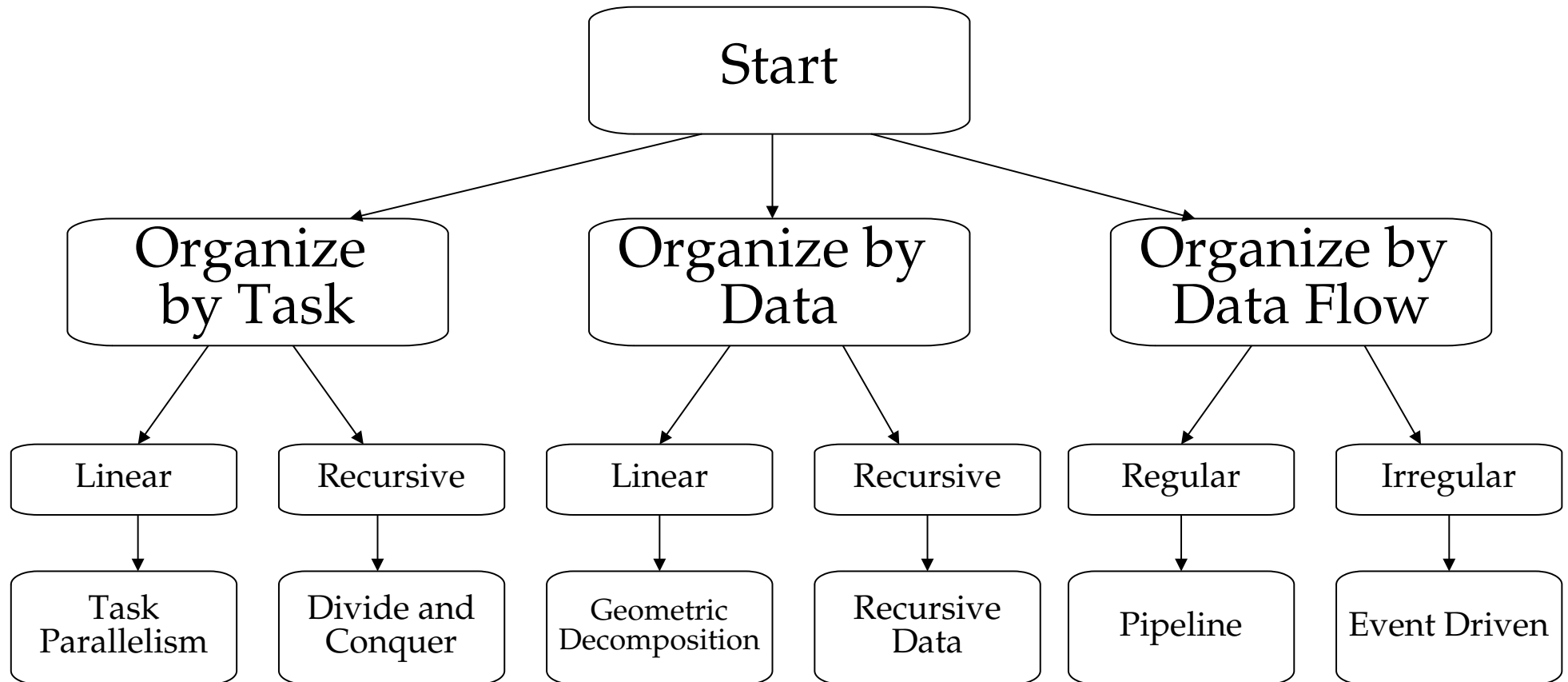
- To find the concurrency in the problem
- **To structure the algorithm to translate concurrency into performance**
- To implement the algorithm in a suitable programming environment
- To execute and tune the performance of the code on a parallel system

Unfortunately, these have not been separated into levels of abstractions that can be dealt with independently.

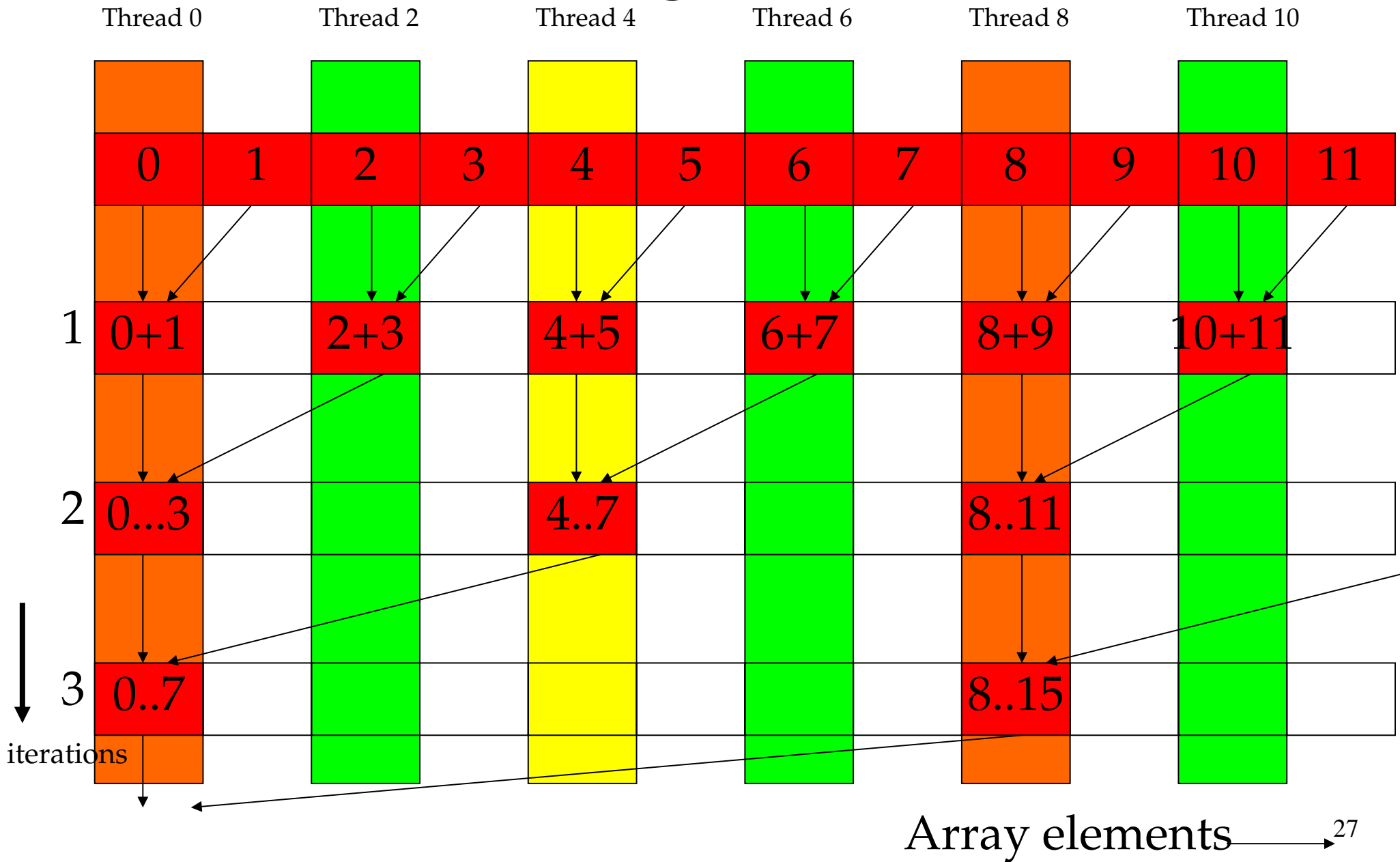
Algorithm

- A step by step procedure that is guaranteed to terminate, such that each step is precisely stated and can be carried out by a computer
 - Definiteness - the notion that each step is precisely stated
 - Effective computability - each step can be carried out by a computer
 - Finiteness - the procedure terminates
- Multiple algorithms can be used to solve the same problem
 - Some require fewer steps
 - Some exhibit more parallelism
 - Some have larger memory footprint than others

Choosing Algorithm Structure

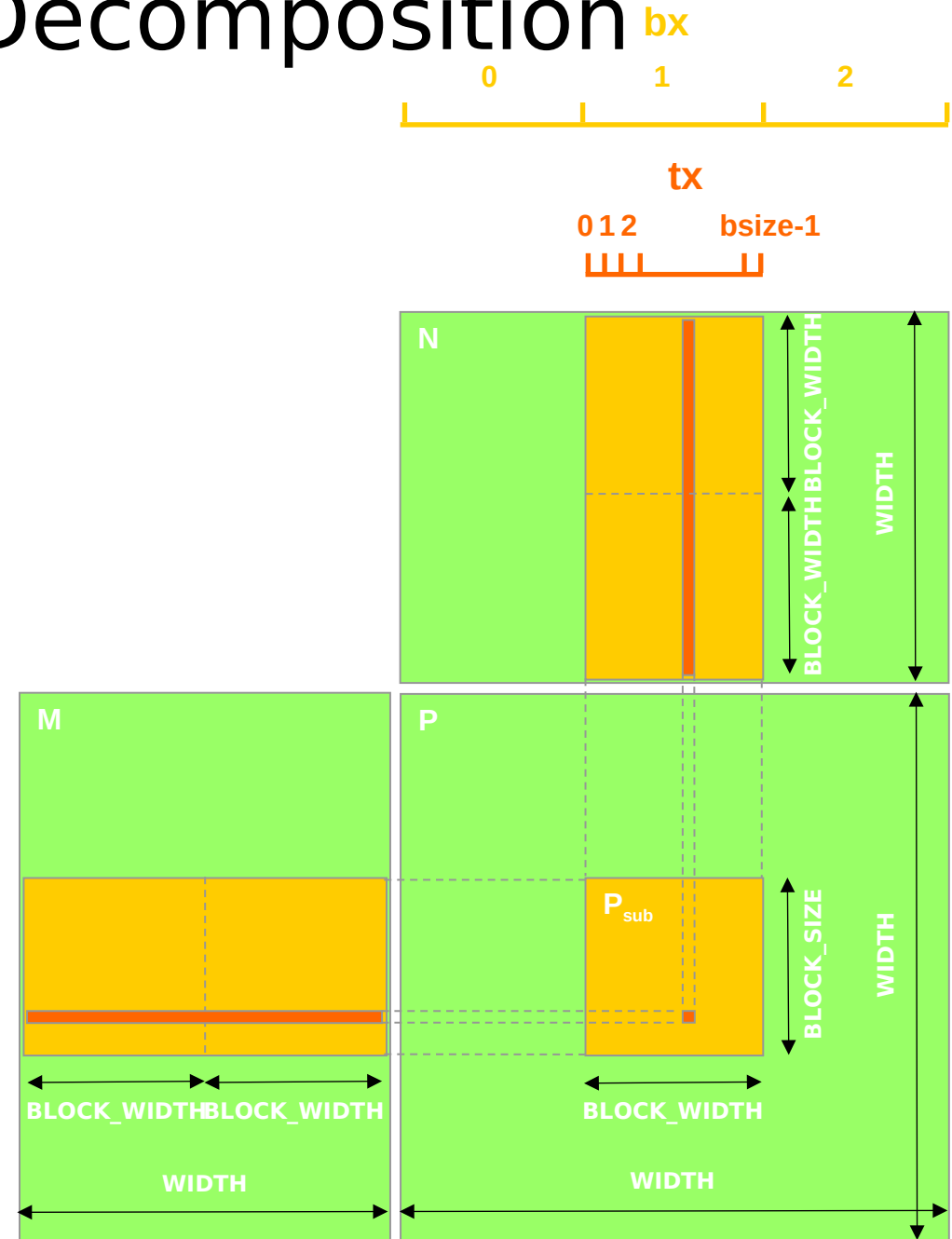


Mapping a Divide and Conquer Algorithm



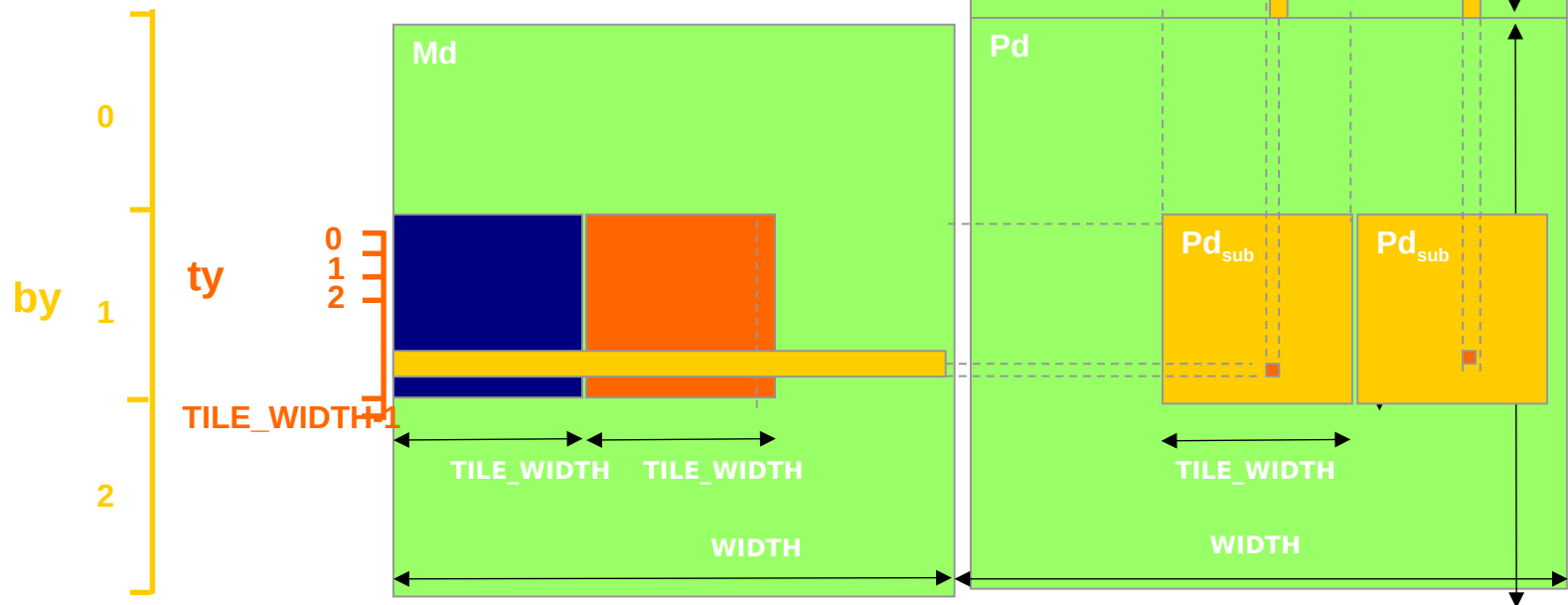
Tiled (Stenciled) Algorithms are Important for Geometric Decomposition

- A framework for memory data sharing and reuse by increasing data access locality.
 - Tiled access patterns allow small cache/scartchpad memories to hold on to data for re-use.
 - For matrix multiplication, a 16X16 thread block perform $2 \times 256 = 512$ float loads from device memory for $256 * (2 \times 16) = 8,192$ mul/add operations.
- A convenient framework for organizing threads (tasks)



Increased Work per Thread for even more locality

- Each **thread** computes two element of Pd_{sub}
- Reduced loads from global memory (Md) to shared memory
- Reduced instruction overhead
 - More work done in each iteration



Double Buffering

- a frequently used algorithm pattern

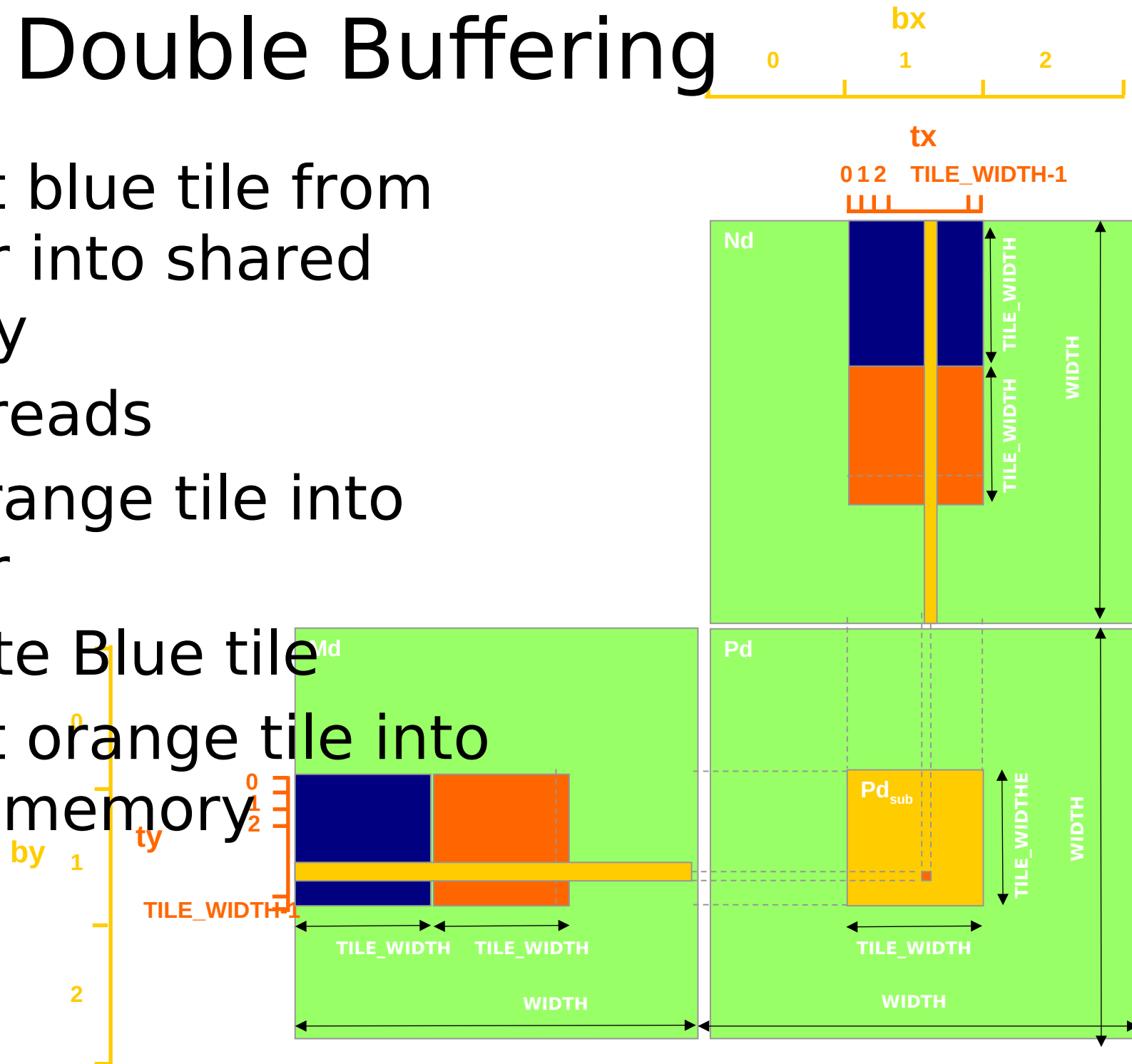
- One could double buffer the computation, getting better instruction mix within each thread
 - This is classic software pipelining in ILP compilers

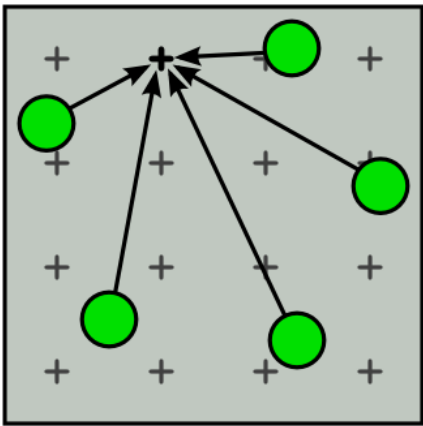
```
Loop {  
    Load current tile to shared memory  
  
    syncthread()  
  
    Compute current tile  
  
    syncthread()  
}
```

```
Load next tile from global memory  
  
Loop {  
    Deposit current tile to shared memory  
  
    syncthread()  
  
    Load next tile from global memory  
  
    Compute current tile  
  
    syncthread()  
}
```

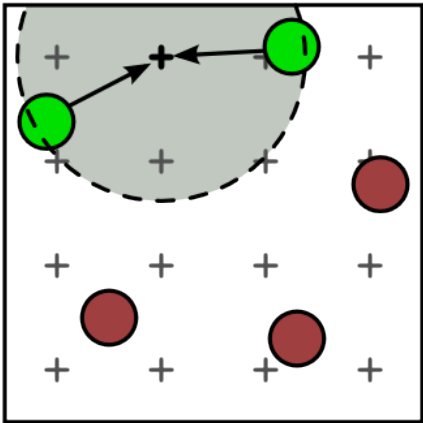
Double Buffering

- Deposit blue tile from register into shared memory
- Syncthread
- Load orange tile into register
- Compute Blue tile
- Deposit orange tile into shared memory
-

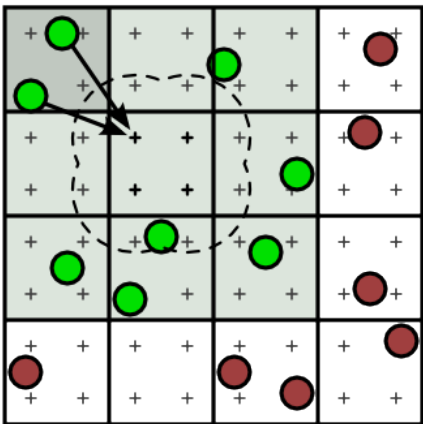




(a) Direct summation
 At each grid point, sum the electrostatic potential from all charges



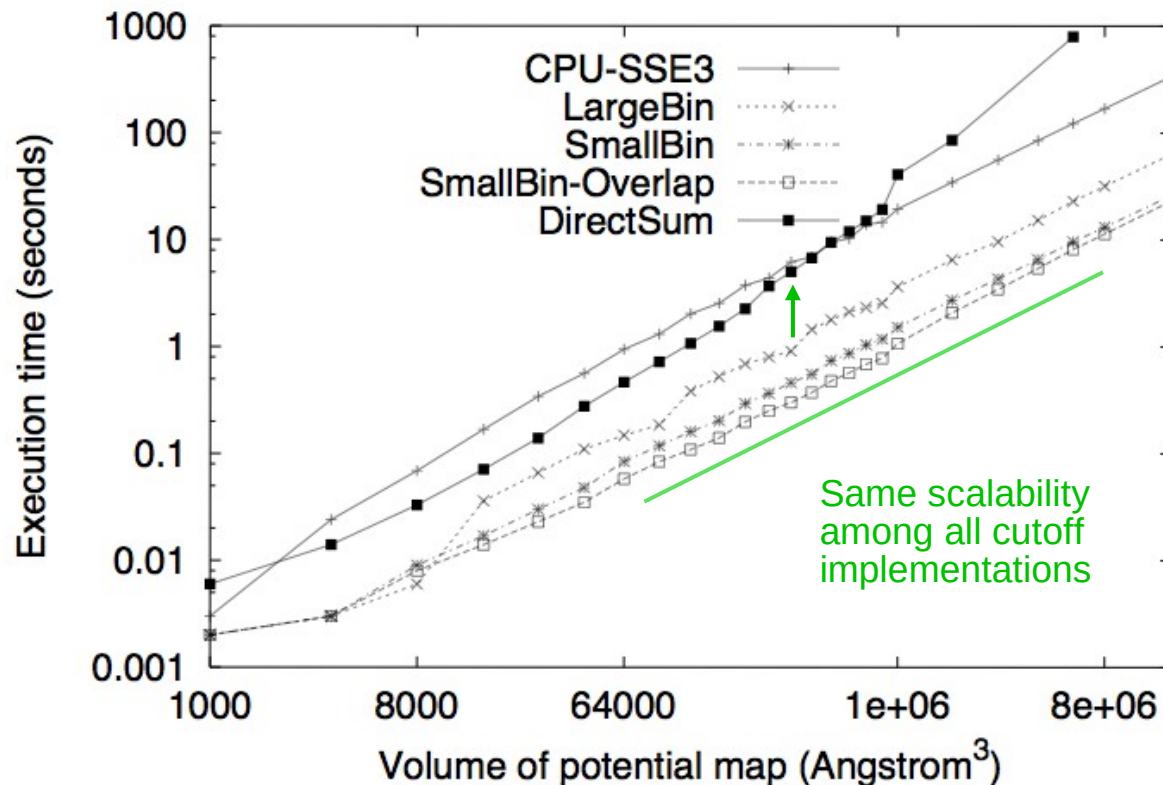
(b) Cutoff summation
 Electrostatic potential from nearby charges summed; spatially sort charges first



(c) Cutoff summation using direct summation kernel
 Spatially sort charges into bins; adapt direct summation to process a bin

Figure 10.2 Cutoff Summation algorithm

Cut-Off Summation Restores Data Scalability



Scalability and Performance of different algorithms for calculating electrostatic potential map.